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Sharp upper bounds for the Laplacian graph eigenvalues ☆

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Abstract

Let $G=(V,E)$ be a simple connected graph and $\lambda_1(G)$ be the largest Laplacian eigenvalue of G. In this paper, we prove that:

1. $\lambda_1(G)=\max\{d_u+m_u : u\in V\}$ if and only if G is a regular bipartite or a semiregular bipartite graph, where d_u and m_u denote the degree of u and the average of the degrees of the vertices adjacent to u, respectively.
2. $\lambda_1(G)=2+\sqrt{(r-2)(s-2)}$ if and only if G is a regular bipartite graph or a semiregular bipartite graph, or a path with four vertices, where $r=\max\{d_u+d_v : uv\in E\}$ and suppose $xy\in E$ satisfies $d_x+d_y=r$, $s=\max\{d_u+d_v : uv\in E-\{xy\}\}$.
3. $$\lambda_1(G)=\max\left\{\frac{d_u(d_u+m_u)+d_v(d_v+m_v)}{d_u+d_v} : uv\in E\right\}$$
   if and only if G is a regular bipartite graph or a semiregular bipartite graph.
4. $\lambda_1(G)\leqslant 2+\sqrt{(t-2)(b-2)}$ with equality if and only if G is a regular bipartite graph or a semiregular bipartite graph, or a path with four vertices, where
   $$t=\max\left\{\frac{d_u(d_u+m_u)+d_v(d_v+m_v)}{d_u+d_v} : uv\in E\right\}$$
   and suppose $xy\in E$ satisfies
   $$\frac{d_x(d_x+m_x)+d_y(d_y+m_y)}{d_x+d_y}=t,$$

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$$b = \max\left\{\frac{d_u(d_u+m_u)+d_v(d_v+m_v)}{d_u+d_v} : uv \in E - \{xy\}\right\}.$$

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1. Introduction

Let $G = (V, E)$ be a simple connected graph on vertex set $V = \{v_1, v_2, \ldots, v_n\}$ and edge set $E = \{e_1, e_2, \ldots, e_m\}$. For any $u \in V$, the degree of u and the average (arithmetic mean) of the degrees of the vertices adjacent to u are denoted by d_u and m_u, respectively. Then $d_u m_u$ is the 2-*degree* of u [6]. Let $D = D(G) = \mathrm{diag}(d_u : u \in V)$ be the diagonal matrix of vertex degrees and let $A = A(G)$ be the adjacency matrix of G. The Laplacian matrix of G is $L(G) = D(G) - A(G)$. From this fact and Geršgorin's theorem, it follows that its eigenvalues are nonnegative real numbers. Moreover, since its rows sum to 0, 0 is the smallest eigenvalue of $L(G)$. Hence we may assume that $\lambda_1(G) \geqslant \lambda_2(G) \geqslant \cdots \geqslant \lambda_{n-1}(G) \geqslant \lambda_n(G) = 0$ are the eigenvalues of $L(G)$.

There are some known upper bounds for $\lambda_1(G)$.

In 1985, Anderson and Morley [1] proved that

$$\lambda_1(G) \leqslant \max\left\{d_u + d_v : uv \in E\right\} \tag{1}$$

with equality holds if and only if G is a regular bipartite graph or a semiregular bipartite graph.

In 1997, Li and Zhang [4] improved the upper bound (1) as follows:

$$\lambda_1(G) \leqslant 2 + \sqrt{(r-2)(s-2)}, \tag{2}$$

where $r = \max\{d_u + d_v : uv \in E\}$ and suppose that $xy \in E$ satisfies $d_x + d_y = r$ and $s = \max\{d_u + d_v : uv \in E - \{xy\}\}$.

In 1998, Merris [6] gave that

$$\lambda_1(G) \leqslant \max\left\{d_u + m_u : u \in V\right\}. \tag{3}$$

In 1998, Li and Zhang [5] presented the following result:

$$\lambda_1(G) \leqslant \max\left\{\frac{d_u(d_u+m_u)+d_v(d_v+m_v)}{d_u+d_v} : uv \in E\right\}. \tag{4}$$

It is easy to see that the upper bound (4) is an improvement of (3). But the extremal graphs which achieve the upper bounds of (2)–(4) were not determined. The aim of this paper is to determine the extremal graphs of the bounds (2)–(4) and to give a new upper bound for $\lambda_1(G)$ (Theorem 2.11), which is lower than (4), and determine its extremal graphs.

2. Lemmas and results

Let M be a nonnegative matrix and $\rho(M)$ be the spectral radius of M.

Lemma 2.1 [3]. *Let $M = (m_{ij})$ be an irreducible nonnegative matrix and let $B = (b_{ij})$ be a complex matrix. Denote $|B| = (|b_{ij}|)$. Assume that $M \geqslant |B|$, i.e., $m_{ij} \geqslant |b_{ij}|$ for any i and j. Then $\rho(M) \geqslant \rho(B)$. If $\rho(M) = \rho(B)$ and if $\lambda = \mathrm{e}^{\mathrm{i}\varphi}\rho(B)$ is an eigenvalue of B, where φ is a real number and $\mathrm{i} = \sqrt{-1}$, then there exist real numbers $\theta_1, \theta_2, \ldots, \theta_n$ such that $B = \mathrm{e}^{\mathrm{i}\varphi}UMU^{-1}$, where $U = \mathrm{diag}(\mathrm{e}^{\mathrm{i}\theta_1}, \mathrm{e}^{\mathrm{i}\theta_2}, \ldots, \mathrm{e}^{\mathrm{i}\theta_n})$.*

Lemma 2.2 [3]. *Let $M = (m_{ij})$ be an $n \times n$ irreducible nonnegative matrix with spectral radius $\rho(M)$, and let $R_i(M)$ be the ith row sum of M, i.e., $R_i(M) = \sum_{j=1}^{n} m_{ij}$. Then*

$$\min\left\{R_i(M) : 1 \leqslant i \leqslant n\right\} \leqslant \rho(M) \leqslant \max\left\{R_i(M) : 1 \leqslant i \leqslant n\right\}. \tag{5}$$

Moreover, if the row sums of M are not all equal, then the both inequalities in (5) *are strict.*

Let $K = D + A$, and let $\rho(K)$ be the spectral radius of K. Clearly, K is a nonnegative, symmetric and irreducible matrix.

Theorem 2.3. *Let $G = (V, E)$ be a connected graph with n vertices. Then $\lambda_1(G) \leqslant \rho(K)$ with equality if and only if G is a bipartite graph.*

Proof. Clearly, $|L| = D + A = K$. Since G is connected, it follows that A and therefore K is irreducible and nonnegative. By Lemma 2.1, $\lambda_1(G) \leqslant \rho(K)$. Now suppose that $\lambda_1(G) = \rho(K)$, then by Lemma 2.1, $D - A = U(D + A)U^{-1}$, where $U = \mathrm{diag}(\mathrm{e}^{\mathrm{i}\theta_1}, \ldots, \mathrm{e}^{\mathrm{i}\theta_n})$, and $\theta_1, \ldots, \theta_n$, are real. Assume that G is not bipartite. Then G has an odd cycle $u_1u_2 \ldots u_{2k}u_{2k+1}u_1$. Hence, $(D - A)_{u_1u_2} = -1 = U_{u_1u_1} \times 1 \times U^{-1}_{u_2u_2}$. So, $U_{u_2u_2} = -U_{u_1u_1}$. Repeating this argument, one can obtain that $U_{u_3u_3} = -U_{u_2u_2} = U_{u_1u_1}, \ldots, U_{u_{2k+1}u_{2k+1}} = U_{u_1u_1}$ and $U_{u_{2k+1}u_{2k+1}} = -U_{u_1u_1}$, impossible. Thus G is bipartite.

Conversely suppose that G is a bipartite graph and S, T is a bipartition of V. Then it is easy to verify that $W(D - A)W^{-1} = D + A$, where $W = \mathrm{diag}(W_{uu} : u \in V)$, and $W_{uu} = 1$ if $u \in S$ and $W_{uu} = -1$ if $u \in T$. Thus $\lambda_1(G) = \lambda_1(D - A) = \rho(D + A) = \rho(K)$. $\square$

A semiregular graph $G = (V, E)$ is a graph with bipartition (V_1, V_2) of V such that all vertices in V_i have the same degree k_i for $i = 1, 2$.

As an application of Theorem 2.3, we now give a new proof of the upper bound (3) for $\lambda_1(G)$ and characterize its extremal graphs.

Theorem 2.4. *Let $G = (V, E)$ be a connected graph. Then*

$$\lambda_1(G) \leqslant \max\left\{d_u + m_u : u \in V\right\}$$

with equality if and only if G is either a regular bipartite graph or a semiregular bipartite graph.

Proof. By Theorem 2.3, $\lambda_1(G) \leqslant \rho(K)$. Moreover, $\rho(K) = \rho(D^{-1}KD)$, and $R_u(D^{-1}KD) = d_u + m_u$ for any $u \in V(G)$. Hence by Lemma 2.2, $\lambda_1(G) \leqslant \max\{d_u + m_u : u \in V\}$.

Now suppose that equality in (3) holds. Then $\lambda_1(G) = \rho(K)$. It follows from Theorem 2.3 that G is bipartite. Moreover, by Lemma 2.2, for any $u, v \in V$, $R_u(D^{-1}KD) = R_v(D^{-1}KD)$, i.e., $d_u + m_u = d_v + m_v$. Hence $d_u^2 + d_u m_u = \sum_{v\sim u}(d_v + m_v) = \sum_{v\sim u} d_v + \sum_{v\sim u} m_v$. By the definition of m_u, we have $d_u m_u = \sum_{v\sim u} d_v$. Hence $d_u^2 = \sum_{v\sim u} m_v$. Assume that S, T is a bipartition of V, and $u \in S$ is a vertex with maximal degree in S. Then for $v \in T$, $d_v m_v = \sum_{w\sim v} d_w \leqslant d_u d_v$. Hence $m_v \leqslant d_u$. So $d_u^2 = \sum_{v\sim u} m_v \leqslant d_u^2$. This shows that $m_v = d_u$ for each neighbor v of u. Thus, for each neighbor v of u, we have $d_v m_v = d_u d_v$, i.e., $\sum_{w\sim v} d_w = \sum_{w\sim v} d_u$. So, $d_w = d_u$ for each neighbor w of v. Observe that $u, w \in S$, and $v \in T$. Since G is connected, one can obtain $d_w = d_u$ for each $w \in S$. Similarly we can show that all the vertices in T have the same degree.

Suppose that G is a regular bipartite graph or a semiregular bipartite graph. Then all the row sums of $D^{-1}(D + A)D$ are equal. By Lemma 2.2, $\rho(K) = \rho(D^{-1}KD) = \max\{d_u + m_u : u \in V\}$. Since G is bipartite, by Theorem 2.3 again, $\lambda_1(G) = \rho(K) = \max\{d_u + m_u : u \in V\}$. □

We denote the vertex-edge incidence matrix of the graph G by $Q = Q(G) = (q_{ve})$, where q_{ve} is defined as follows:

$$q_{ve} = \begin{cases} 1 & \text{if } v \text{ is on edge } e, \\ 0 & \text{otherwise.} \end{cases}$$

In the sequel, we denote by $\lambda_1(M)$ the spectral radius of M, if M is a square matrix.

Lemma 2.5. *Let G be a simple connected graph. then*

$$\lambda_1(G) \leqslant \lambda_1(Q^{\mathrm{T}}Q)$$

with equality if and only if G is a bipartite graph.

Proof. It is easy to see that $QQ^{\mathrm{T}} = D + A = K$. Recall that $Q^{\mathrm{T}}Q$ and QQ^{T} share the same nonzero eigenvalues. By Theorem 2.3, then $\lambda_1(G) \leqslant \lambda_1(K) = \lambda_1(QQ^{\mathrm{T}}) = \lambda_1(Q^{\mathrm{T}}Q)$.

It is clear that $\lambda_1(G) = \lambda_1(Q^{\mathrm{T}}Q)$ if and only if $\lambda_1(G) = \lambda_1(QQ^{\mathrm{T}}) = \lambda_1(K)$. From Theorem 2.3, we know that $\lambda_1(G) = \lambda_1(Q^{\mathrm{T}}Q)$ if and only if G is a bipartite graph. □

Denote the line graph of G by L_G and let B_L be the adjacency matrix of L_G.

Lemma 2.6 [2, Theorem 2.4.1.]. *Let G is a graph with n vertices and m edges. Then*

$$Q^{\mathrm{T}}Q = 2I_m + B_L.$$

For a given $n \times n$ matrix $A = (a_{ij})$, denote

$$R_i = \sum_{j \neq i} |a_{ij}| \quad \textit{for each } i = 1, 2, \ldots, n,$$

$$S_{ij} = \left\{ z \in C : |z - a_{ii}||z - a_{jj}| \leqslant R_i R_j \right\} \quad \textit{for all } i \neq j,$$

and $S = \bigcup_{i<j} S_{ij}$, where C is the complex number field. In addition, λ denote an eigenvalue of A.

Lemma 2.7 [3]. *Let $A = (a_{ij})$ be a complex matrix of order $n \geqslant 2$. Then the eigenvalues of the matrix A lie in the region of the complex plane determined by the union of the ovals*

$$S_{ij} = \left\{ z : |z - a_{ii}||z - a_{jj}| \leqslant R_i R_j \right\}, \quad (i, j = 1, 2, \ldots, n;\ i \neq j).$$

Lemma 2.8 [4]. *Let A be an irreducible matrix which has two rows such that each of these rows contains at least two nonzero off-diagonal entries. If λ lies on the boundary of S, then λ is a boundary point of each S_{ij}.*

Now we give a new proof of the upper bound (2) and determine its extremal graphs.

Theorem 2.9. *Let $G = (V, E)$ be a connected graph with m edges. Then*

$$\lambda_1(G) \leqslant 2 + \sqrt{(r-2)(s-2)}$$

with equality holds if and only if G is a regular bipartite graph or a semiregular bipartite graph, or a path with four vertices, where $r = \max\{d_u + d_v : uv \in E\}$ and suppose $xy \in E$ satisfies $d_x + d_y = r$, $s = \max\{d_u + d_v : uv \in E - \{xy\}\}$.

Proof. By Lemma 2.7, $\lambda_1(B_L) \leqslant \sqrt{(r-2)(s-2)}$. Therefore from Lemma 2.6, it follows that $\lambda_1(Q^{\mathrm{T}}Q) \leqslant 2 + \sqrt{(r-2)(s-2)}$. Hence $\lambda_1(G) \leqslant \lambda_1(Q^{\mathrm{T}}Q) \leqslant 2 + \sqrt{(r-2)(s-2)}$.

Now suppose that equality in (2) holds. Then $\lambda_1(G) = \lambda_1(Q^{\mathrm{T}}Q)$. By Lemma 2.5, G is bipartite. Moreover, $\lambda_1(B_L) = \sqrt{(r-2)(s-2)}$. Since G is connected, the line graph L_G is connected; therefore B_L is irreducible. If B_L has two rows such that each of these rows contains at least two nonzero off-diagonal entries. Then by Lemma 2.8, $\lambda_1(B_L)$ is a boundary point of each S_{ij} of B_L. Hence

$$\lambda_1(B_L) = \sqrt{(r-2)(s-2)} = \sqrt{R_i(B_L)R_j(B_L)}, \quad 1 \leqslant i < j \leqslant m.$$

Therefore all the row sums of B_L are equal. Namely, L_G is regular. Hence G is regular bipartite or semiregular bipartite. If B_L has exactly one row which contains at least two nonzero off-diagonal entries, then L_G has exactly one vertex e_i such that e_i and all other vertices e_j are adjacent. Thus G is a path with four vertices. If B_L has no rows with more than one off-diagonal entries, then G is a path with two or three vertices, which are regular bipartite and semiregular bipartite, respectively.

It is easy to verify that equality in (2) is satisfied by: regular bipartite graphs, semiregular bipartite graphs and path with four vertices. $\square$

The following theorem gives a new proof of (4) and the necessary and sufficient conditions for the holding of the equality in (4).

Theorem 2.10. *Let $G = (V, E)$ be a connected graph. Then*

$$\lambda_1(G) \leqslant \max\left\{\frac{d_u(d_u+m_u)+d_v(d_v+m_v)}{d_u+d_v} : uv \in E\right\}$$

with equality holds if and only if G is a regular bipartite graph or a semiregular bipartite graph.

Proof. Let $N = T^{-1}(B_L + 2I)T = T^{-1}B_L T + 2I$, where B_L is the adjacency matrix of the line graph L_G, T is the sum of the diagonal degree matrix of L_G and $2I$, which has the same row index and column index as B_L. By the definition of the line graph of graph G, if uv is an edge of G, then it is an vertex of L_G. Therefore the corresponding row sum of N is

$$\frac{\sum\limits_{x\sim u}(d_x+d_u) + \sum\limits_{y\sim v}(d_y+d_v)}{d_u+d_v} = \frac{d_u(d_u+m_u)+d_v(d_v+m_v)}{d_u+d_v},$$

where $u \sim v$ means that u and v in G are adjacent.

By Lemma 2.2,

$$\lambda_1(N) \leqslant \max\left\{\frac{d_u(d_u+m_u)+d_v(d_v+m_v)}{d_u+d_v} : uv \in E\right\}.$$

From Lemmas 2.5 and 2.6, $\lambda_1(G) \leqslant \lambda_1(B_L + 2I) = \lambda_1(N)$. Hence

$$\lambda_1(G) \leqslant \max\left\{\frac{d_u(d_u+m_u)+d_v(d_v+m_v)}{d_u+d_v} : uv \in E\right\}.$$

Now suppose that equality in (4) holds. Then $\lambda_1(G) = \lambda_1(N) = \lambda_1(B_L + 2I) = \lambda_1(Q^{\mathrm{T}}Q)$. From Lemma 2.5, G is bipartite.

By Lemma 2.2, if

$$\lambda_1(N) = \max\left\{\frac{d_u(d_u+m_u)+d_v(d_v+m_v)}{d_u+d_v} : uv \in E\right\},$$

then all the row sums of N are equal, i.e.,

$$\max\left\{\frac{d_u(d_u+m_u)+d_v(d_v+m_v)}{d_u+d_v}:uv\in E\right\}$$
$$=\min\left\{\frac{d_u(d_u+m_u)+d_v(d_v+m_v)}{d_u+d_v}:uv\in E\right\}=\lambda_1(N).$$

Assume that V_1, V_2 is a bipartition of V. Since G is connected, for any two vertices $u\in V_1$, $v\in V_2$, there is a path $uv_1u_2v_2,\ldots,u_{k-1}v_{k-1}u_kv$ joining u and v. Therefore

$$\begin{aligned}
&\frac{d_u(d_u+m_u)+d_{v_1}(d_{v_1}+m_{v_1})}{d_u+d_{v_1}}\\
&\quad=\frac{-\big(d_{v_1}(d_{v_1}+m_{v_1})+d_{u_2}(d_{u_2}+m_{u_2})\big)}{-(d_{v_1}+d_{u_2})}\\
&\quad=\cdots\\
&\quad=\frac{-\big(d_{v_{k-1}}(d_{v_{k-1}}+m_{v_{k-1}})+d_{u_k}(d_{u_k}+m_{u_k})\big)}{-(d_{v_{k-1}}+d_{u_k})}\\
&\quad=\frac{d_{u_k}(d_{u_k}+m_{u_k})+d_v(d_v+m_v)}{d_{u_k}+d_v}=\lambda_1(G).
\end{aligned}$$

Then it follows from the theorem of ratio of equality that

$$\lambda_1(G)=\frac{d_u(d_u+m_u)+d_v(d_v+m_v)}{d_u+d_v}\quad\text{for any } u\in V_1,\ v\in V_2.$$

In the sequel, we shall show that for any $u\in V$, d_u+m_u is equal. Then we can deduce that G is regular bipartite or semiregular bipartite from the proof of Theorem 2.4.

Clearly,

$$\frac{d_u(d_u+m_u)+d_v(d_v+m_v)}{d_u+d_v}$$

is the weighted average of d_u+m_u and d_v+m_v, d_u and d_v are the weights, respectively. Assume that $d_v+m_v\leqslant d_u+m_u$, then

$$d_v+m_v\leqslant\frac{d_u(d_u+m_u)+d_v(d_v+m_v)}{d_u+d_v}\leqslant d_u+m_u$$

with equality holds on either side if and only if $d_u+m_u=d_v+m_v$.

If there exist two vertices $u\in V_1$ and $v\in V_2$ such that $d_v+m_v<d_u+m_u$, then by the implication of weighted average, we know

$$d_v+m_v<\lambda_1(G)=\frac{d_u(d_u+m_u)+d_v(d_v+m_v)}{d_u+d_v}<d_u+m_u.$$

Since

$$\lambda_1(G) = \frac{d_u(d_u + m_u) + d_x(d_x + m_x)}{d_u + d_x} = \frac{d_v(d_v + m_v) + d_y(d_y + m_y)}{d_v + d_y},$$

we may conclude that $d_x + m_x < \lambda_1(G) < d_y + m_y$, for any $x \in V_2$ and $y \in V_1$. Let $N(x)$ denote the set of vertices adjacent to x. Choose a vertex i with minimal degree in V_1, and choose a vertex j with maximal degree in $N(i)$. Then $d_i + m_i \leqslant d_j + m_j$, a contradiction. Similarly we can show that $d_v + m_v > d_u + m_u$ is also not possible.

Therefore, for any two vertices $u \in V_1$ and $v \in V_2$, we have $d_u + m_u = d_v + m_v$. Since G is connected, we know that for any $v \in V$, $d_v + m_v$ is equal. Hence G must be regular bipartite or semiregular bipartite.

It is easy to verify that the equality in (4) holds for all the graphs: regular bipartite graphs and semiregular bipartite graphs. □

Now we give a new upper bound for $\lambda_1(G)$ in the following Theorem 2.11, which is an improvement of (4).

Theorem 2.11. *Let G be a connected graph with m edges. Then*

$$\lambda_1(G) \leqslant 2 + \sqrt{(t-2)(b-2)}$$

with equality holds if and only if G is a regular bipartite graph or a semiregular bipartite graph, or a path with four vertices, where

$$t = \max\left\{\frac{d_u(d_u + m_u) + d_v(d_v + m_v)}{d_u + d_v} : uv \in E\right\},$$

and suppose $xy \in E$ satisfies

$$\frac{d_x(d_x + m_x) + d_y(d_y + m_y)}{d_x + d_y} = t,$$

$$b = \max\left\{\frac{d_u(d_u + m_u) + d_v(d_v + m_v)}{d_u + d_v} : uv \in E - \{xy\}\right\}.$$

Proof. As the proof of Theorem 2.10, let $N = T^{-1}(B_L + 2I)T = T^{-1}B_L T + 2I$. And let $M = T^{-1}B_L T$. From Lemma 2.7, $\lambda_1(M) \leqslant \sqrt{(t-2)(b-2)}$. Thus $\lambda_1(G) \leqslant \lambda_1(N) = 2 + \lambda_1(M) \leqslant 2 + \sqrt{(t-2)(b-2)}$.

Now suppose that $\lambda_1(G) = 2 + \sqrt{(t-2)(b-2)}$. Then $\lambda_1(G) = \lambda_1(N) = \lambda_1(B_L + 2I)$. By Lemmas 2.5 and 2.6, G is bipartite.

If $\lambda_1(G) = 2 + \sqrt{(t-2)(b-2)}$, then $\lambda_1(M) = \sqrt{(t-2)(b-2)}$. Now if M has two rows such that each of these rows contains at least two nonzero off-diagonal entries (in fact, M has at least three rows), then by Lemma 2.8, $\lambda_1(M)$ is an boundary point of each S_{ij} of M. Hence

$$\lambda_1(M) = \sqrt{(t-2)(b-2)} = \sqrt{R_i(M)R_j(M)}, \quad 1 \leqslant i < j \leqslant m.$$

Therefore, all the row sums of M, and hence of N are equal. From the proof of Theorem 2.10, we know that G is regular bipartite or semiregular bipartite. And if M, and hence B_L has exactly one row which contains at least two nonzero off-diagonal entries. Then L_G is a star graph, Therefore, G must be a path with four vertices. If M, and hence B_L has no rows with more than one off-diagonal entries, then G is a path with two or three vertices, which are regular bipartite and semiregular bipartite, respectively.

Conversely, it is easy to verify that the equality holds for: regular bipartite graphs, semiregular bipartite graphs or the path with four vertices. $\square$

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